Exposure and Fate Assessment Screening Tool (E-FAST)
Beta Version
Documentation Manual

Prepared for:

U.S. Environmental Protection Agency
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1. INTRODUCTION

What is E-FAST?

The Exposure and Fate Assessment Screening Tool, also known as E-FAST, is a "screening level" computer tool that allows the user to generate estimates of chemical concentrations in water to which aquatic life may be exposed and estimates of human inhalation and drinking water exposures (potential dose rates) resulting from chemical releases to air, water, and land. E-FAST can also be used to assess inhalation and dermal exposures to chemicals that may result from use of certain types of consumer products. The exposed population is either some segment of the general population or consumers. Exposures to workers in occupational settings are not assessed in this model.

E-FAST was developed as a screening level tool to support the Environmental Protection Agency (EPA) assessments of the potential exposures to new chemicals which are submitted to EPA under Section 5 of the Toxic Substances Control Act (TSCA). It should be noted that screening level tools are rarely, if at all, used as the sole justification for regulatory decision making at EPA. Additional data and more rigorous tools are used to improve the estimates of exposures and risks for such decisions. Thus, although the use of E-FAST may be very useful to manufacturers of new chemicals, its results may not accurately reflect all of the information and data used by EPA to make a regulatory decision on a new chemical.

Because, by definition, commercial manufacture of TSCA Section 5 new chemicals has not commenced when EPA conducts its TSCA Section 5 assessments, measured data on surface water concentrations and human exposures are not available. The exposure scenarios in E-FAST contain default exposure parameter values which allow the exposures to be estimated with minimal data entry. The assumptions and calculations used in the exposure scenarios are explained in Sections 2 through 5 of this document. It should be noted that because E-FAST incorporates either a combination of upper percentile and mean exposure parametric values or all upper percentile parametric values as defaults, the potential dose rate estimates are considered "high end to bounding" estimates.

When Should I Use the Model?

E-FAST is appropriate for use as a screening level tool to assess potential dose rates resulting from chemical discharges to air (stack or fugitive releases), surface water, or land. E-FAST can also be used to estimate potential inhalation and dermal dose rates to chemical components of consumer products. These products include hard surface cleaners, soaps, air fresheners, paints, gasoline, and motor oil.

When is it Not Appropriate to Use the Model?

E-FAST is characterized by EPA as a "screening model." Screening model results are intended to be conservative estimates because predicted concentrations and exposures are likely to be higher, or at least higher than average, as compared to concentrations and exposures that might actually be occurring in a real world setting. If a predicted exposure is found to result in an unacceptably high health risk with a screening model, then an appropriate next step in the assessment process is to refine the parameter input and/or to perform the assessment with more sophisticated and perhaps more complex models. Another response might be to consider monitoring to confirm results of the model.

E-FAST does not estimate physical-chemical properties, environmental fate parameters, environmental releases, worker exposures, and consumer exposures to products not covered under TSCA. If measured physical-chemical and environmental fate data do not exist, commercially available estimation software can be used to estimate these properties. Environmental releases and worker exposures can be estimated using the ChemSTEER model, which is publicly available from EPA. To obtain this software, contact Scott Prothero (202-260-1566) in EPA's Office of Pollution Prevention and Toxics (OPPT).

The exposures estimated in E-FAST are potential dose rates (PDR). PDRs are the predicted amounts of chemical inhaled, ingested, or on the surface of the skin. E-FAST does not estimate absorbed doses via inhalation or ingestion. E-FAST does have an option to estimate absorbed dermal doses, if the user provides the dermal permeability coefficient for the chemical being assessed.

How Does E-FAST Relate to Previous DOS-Based Tools Developed by OPPT?

E-FAST replaces the following DOS-based OPPT tools: SEAS, DERMAL, SCIES, PDM3, the SIDS database, and FLUSH.

What Computer Hardware and Software Do I Need to Run the E-FAST Model?

- Processor - 486 computer (pentium or faster recommended)
- Memory - 16 MB
- Hard disk space - 48 MB
- Operating system - Windows 95, Windows 98, or Windows NT
- Screen resolution - SVGA: 800 x 600
- Color setting - high color (16 bit) (functions on 256 color; however, harder to view)
- Creates reports in WordPerfect (Versions 6.1 - 8.0). This software is needed in order to combine reports
- Printer for printing reports
- Mouse

What Information Do I Need to Run the E-FAST Model?

The required information is listed below. Depending on the media of release, some of these parameters may not apply to your chemical.

All Media

- Estimated releases to air, water, and land (mass/time)
- Frequencies and durations of release events (e.g., days/year)

Releases to Water

- Removal in wastewater treatment (%)
- Removal in drinking water treatment (if known) (%)
- Estimated fraction that will sorb to sludge and remain with sludge going to land application (unitless)
- Bioconcentration factor [(mg/kg)/(mg/L)]
- Concentration of concern (μg/L) (i.e., acute and/or chronic concern level for protection of aquatic life)

Releases to Land

- Estimated potential for migration to groundwater from land disposal (estimated from physical-chemical properties and physical form of the disposed material)

Releases to Air

- Estimated removal by air pollution control devices or by incineration (%)

Chemicals Present in Consumer Products

- Molecular weight
- Weight fraction in consumer products (if applicable)
- Measured or estimated vapor pressure of the chemical (torr)

In addition to the required information listed above, the calculation procedures in E-FAST also require other exposure parameter information concerning body weights, intake rates, etc. Default values for each of these parameters are provided in the model for three population groups (adults, children, and infants) and two exposure types (acute and chronic for adults; acute only for children and infants), where appropriate. Most of these default values are conservative in nature and are the "recommended" values in EPA's *Exposure Factors Handbook* (U.S. EPA, 1997). These default values can be changed by the user. The E-FAST default exposure parameter values are presented in Table 1-1.

How Do I Use the Model?

E-FAST consists of several exposure assessment modules organized by type of release (e.g., industrial releases, household releases, and consumer products) and the environmental medium to which the chemical is released. The model directs the user through the process of identifying release sites and media of release, entering chemical properties and environmental fate values, and estimating concentrations in environmental media and potential human and aquatic life exposures.

At the first screen, the user can select one of four modules: General Population Exposure from Industrial Releases, Down the Drain (i.e., releases to surface water from use of consumer products), Consumer Exposure, and Aquatic Environment Exposure/Risk. These modules are described in the following sections of this documentation manual.

Table 1-1. Default Exposure Parameter Values Used in E-FAST

Exposure Parameter	Population	Exposure Type	Default Value	Source	Comment
Body Weight	Adult	All	71.8 kg	U.S. EPA (1997)	Mean adult body weight (EFH Table 7-11)
	Child	All	26.9 kg	U.S. EPA (1997)	Average of mean body weights for children aged 2 to 12 (EFH Table 7-3)
	Infant	All	10.2 kg	U.S. EPA (1997)	Average of mean body weights for infants aged 6 months to 2 years (EFH Table 7-3)
Drinking Water Intake	Adult	Chronic	1.4 L/day	U.S. EPA (1997)	Mean adult ingestion rate (EFH Table 3-30)
	Adult	Acute	6 L/day	U.S. EPA (1997)	Ingestion rate for active adults in temperate climates (EFH Table 3-30)
	Child	Acute	1.5 L/day	U.S. EPA (1997)	95th percentile ingestion rate for children aged 1 to 10 (EFH Table 3-30)
	Infant	Acute	0.76 L/day	U.S. EPA (1997)	95th percentile ingestion rate for children less than 1 year old (EFH Table 3-30)
Inhalation Rate	Adult	Chronic	13.3 m^3/day	U.S. EPA (1997)	Average of adult male and female means (EFH Table 5-23)
	Adult	Acute	see comment		For consumer exposures--1.1 m^3/hr during product use and 0.55 m^3/hr after product use
	Child	Acute	9.6 m^3/day	U.S. EPA (1997)	For consumer exposures--Average of mean values for age groups from 1 to 11 years (EFH Table 5-23) (avg = 0.36 m^3/hr)
	Infant	Acute	4.5 m^3/day	U.S. EPA (1997)	For consumer exposures--Mean value for infants less than 1 year old (EFH Table 5-23) (avg = 0.19 m^3/hr)
Fish Ingestion Rate	Adult	Chronic	6.0 g/day	U.S. EPA (1997)	Long term general population average ingestion of freshwater/estuarine fish (EFH Table 10-81)
	Adult	Acute	129 g/day	U.S. EPA (1997)	Mean serving size for general population (EFH Table 10-82)
	Child	Acute	89 g/day	U.S. EPA (1997)	Average of mean 1-day intakes for age 6 -11, consumers only (EFH Table 10-46)
	Infant	Acute	67 g/day	U.S. EPA (1997)	Average of mean 1-day intakes for ages 5 and under, consumers only (EFH Table 10-46)
Non-Carcinogenic Averaging Times	Adult	Chronic	30 years	U.S. EPA (1997)	For ambient exposures--95th percentile residential occupancy value (EFH Table 15-176)
	Adult	Chronic	57 years		For consumer exposures--Active usage of consumer products during years 18 to 75.
	Adult	Acute	1 day		
	Child	Acute	1 day		
	Infant	Acute	1 day		
Carcinogenic Averaging Time	All	NA	75 years	U.S. EPA (1997)	Average life expectancy of general population (EFH page 8-1)

2. GENERAL POPULATION EXPOSURE FROM INDUSTRIAL RELEASES

2.1 Releases to Surface Water from Manufacturing, Processing, and Industrial Use Sites

Wastewaters generated by manufacturing, processing, and industrial and commercial use are typically sent to on-site treatment or are sent to Publicly Owned Treatment Works (POTWs) prior to release to surface waters. Using physical-chemical property data and estimates of biodegradability, the effectiveness of the treatment can be estimated, so that the amount actually getting through to the receiving water body can be predicted. The receiving water will dilute the discharge from the facility or the POTW, and an in-stream concentration of the chemical can be calculated using stream flow information. Stream in this context means the receiving body of water, and includes creeks and rivers as well as bays, estuaries, and oceans.

Since in-stream concentrations will vary with the stream flow, there may be periods of lower flow conditions when the same amount released on a regular basis may cause problems. E-FAST relies on historical stream flow data to predict how often this will happen under "local" and "generic" exposure settings.

> *Local Exposure:* E-FAST contains a database of stream flow values obtained from the Gage File maintained in EPA's STORET system. For those cases in which the discharge location is known, the flows can be located by typing in the National Pollutant Discharge Elimination System (NPDES) number. This is the state code followed by a seven-digit number. If the NPDES number is not available, then the facilities can be located by facility name, Standard Industrial Classification (SIC) Code, or REACH Number.

> *Generic Exposure (when the discharge sites are unknown):* Just as there are variations in facility sizes, there are variations in stream flows. Additionally, stream flows vary with time. The impact of this on the assessment is that more than one concentration needs to be calculated. In order to assess generic exposures to releases from a particular type of facility or facilities, the user must determine to which SIC code the facility or facilities belongs.[1] E-FAST contains data on receiving stream flows for facilities with the SIC codes most commonly encountered in new chemical submissions under Section 5 of TSCA. The stream flows for "POTW, Industrial" can be selected to represent industrial uses not represented in the list of SIC codes in E-FAST. The stream flows for "POTW, All" can be selected for commercial uses not shown in the SIC-code list.

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[1] The SIC system was developed in the 1930s for use in the classification of establishments by types of activity in which they are primarily engaged. The SIC system has been periodically revised since its inception to reflect the economy's changing industrial composition and organization. The last revision of the SIC was in 1987. In 1998, the Office of Management and Budget released the North American Industry Classification System (NAICS) which is intended to replace the SIC system over a period of years beginning in 1999 (U.S. OMB, 1998). The classification system currently used by E-FAST is the 1987 SIC system.

Because the stream flow data used in E-FAST are estimated flows at the downstream end of specific stream segments, the estimated stream flow for any given stream segment presumably includes the discharge flow from any facility on that segment. For large streams this is not an important consideration, but for facilities on small streams, this may result in underestimates of actual streamflows. For example, the discharge from a facility with a discharge flow of 10 million liters per day releasing to a stream which has an estimated low flow of 10 million liters per day is not insignificant; the discharge flow is assumed in E-FAST to constitute all of the receiving stream's flow. Based on the available data, there are a significant number of facilities for which the facility discharge flow constitutes a large fraction of the stream flow under low flow conditions.

2.1.1 Estimation of Surface Water Concentrations

2.1.1.1 *Estimation of Surface Water Concentrations in Rivers and Streams*

E-FAST uses the following formula to calculate surface water concentrations in free-flowing rivers and streams:

SWC (ppb) = [Release * CF1 * (1 - WWT/100)] / [Stream flow * CF2] (Eqn. 2-1)

where:

SWC	=	Surface water concentration (parts per billion or µg/liter);
Release	=	Chemical release to wastewater (i.e., pre-treatment release) (kilograms/site/day);
CF1	=	Conversion factor from kilograms to micrograms (10^9);
WWT	=	Removal in wastewater treatment (%);
WWT/100	=	Converts wastewater treatment efficiency from a percentage to a fraction;
Stream flow	=	Measured or estimated flow of the receiving stream (million liters per day (MLD)); and
CF2	=	Conversion factor from MLD to L/day (10^6).

This equation is valid for both site-specific and SIC-code (generic) release situations. SIC-code analyses are performed when the locations of chemical release are unknown or when there are no available stream flow data for the receiving stream.

Site-specific surface water concentrations are calculated from measured or estimated arithmetic mean and 7Q10 flows obtained from the GAGE File in EPA's STORET system. Harmonic mean, 30Q5, and 1Q10 flows are calculated from the equations presented below (Versar, 1992a). The units of flow input to these equations are million liters per day (MLD). The factor 0.409 is used to convert MLD to units of cubic feet per second (cfs) (e.g., cfs/MLD). Receiving stream flows for SIC-code release situations were developed using the Stream Dilution Factor Program (SDFP) (Versar, 1998).

Harmonic Mean (HM): stream flows are used to generate estimates of chronic human exposures via drinking water and fish ingestion.

$$HM = (1.194) \times \frac{[\ CF \times AMF\ ]^{0.473} \times [\ CF * 7Q10\ ]^{0.552}}{CF} \qquad \text{(Eqn. 2-2)}$$

where,

CF	=	Conversion factor from MLD to cfs (0.409);
HM	=	Harmonic mean flow; and
AMF	=	Arithmetic mean flow.

30Q5 (thirty consecutive days of lowest flow over a five-year period): stream flows are used to generate estimates of acute human exposures via drinking water and fish ingestion.

$$30Q5 = (1.782) \times \frac{[\ 0.409\ cfs/MLD) \times (7Q10)\ ]^{0.966}}{(0.409\ cfs/MLD)} \qquad \text{(Eqn. 2-3)}$$

7Q10 (seven consecutive days of lowest flow over a ten-year period): stream flows are used to generate estimates of exceedances of chronic concentrations of concern for aquatic life.

1Q10 (single day of lowest flow over a ten-year period): stream flows are used to determine if there are acute ecological concerns.

$$1Q10 = (0.843) \times \frac{[\ (0.409\ cfs/MLD) \times (7Q10)\ ]^{0.993}}{(0.409\ cfs/MLD)} \qquad \text{(Eqn. 2-4)}$$

What this equation does: Equation 2-1 estimates chemical concentrations in flowing bodies of water such as rivers and streams. Chemical release to wastewater and estimated removal in wastewater treatment are input values to this equation. The conversion factor of 10^9 converts the chemical release from kg to μg. This value is then divided by the stream flow in MLD; the conversion factor of 10^6 converts MLD to L/day. The results of this equation are chemical concentrations in units of μg/L. For very dilute aqueous solutions (such as surface water concentrations predicted by E-FAST), the units of μg/L and parts per billion (ppb) can be considered equivalent.

2.1.1.2 *Estimation of Surface Water Concentrations in Bays, Lakes and Estuaries*

E-FAST uses the following formula to calculate surface water concentrations in water bodies such as bays, lakes, and estuaries.

$$SWC = \frac{Release\ (kg/site/day) * (1 - WWT/100) * CF1}{Plant\ flow\ (MLD) * CF2 * Dilution\ Factor} \qquad \text{(Eqn. 2-5)}$$

where:

SWC	=	Surface water concentration (ppb or μg/L);

Release	=	Chemical release to wastewater (i.e., pre-treatment release) (kilograms/site/day);
CF1	=	Conversion factor from kg to μg (10^9);
CF2	=	Conversion factor from MLD to L/day (10^6);
WWT	=	Removal in wastewater treatment (%);
WWT/100	=	Converts wastewater treatment efficiency from a percentage to a fraction;
Plant flow	=	Effluent flow of the discharging facility (MLD); and
Dilution factor	=	Acute or chronic dilution factor used for the water body (typically between 1 and 200).

What this equation does: This equation estimates chemical concentrations in water bodies such as bays and estuaries. Chemical release to wastewater is converted to an effluent release by accounting for wastewater treatment removal. The effluent release is divided by the plant flow to generate an effluent concentration. No simple stream flow value represents dilution in these types of water bodies. To account for further dilution in the waterbody, dilution factors for the waterbody of interest are used. Measured dilution factors are typically between 1 (representing no dilution) and 200 and are based on NPDES permits or State regulatory policy. Acute dilution factors are used to develop potential acute dose rates (ADR_{pot}) and chronic dilution factors are used for potential average daily doses (ADD_{pot}) and lifetime average daily doses ($LADD_{pot}$). If an acute dilution factor is available but a chronic dilution factor is not available, then the chronic value is assumed to be equal to the acute value. If a chronic value is available but no acute value is available, then the acute value is assumed to be one.

2.1.2 Estimation of Drinking Water and Fish Ingestion Exposures

Many public water supplies are drawn from the local streams and rivers. As a default assumption, E-FAST conservatively assumes that the estimated concentration in the stream is the concentration that people will ingest; E-FAST allows the user to replace this default assumption.

Since there are many chemicals which accumulate in living organisms (bioaccumulation), the amount of the chemical to which an individual may be exposed from eating fish living in the same streams and rivers is calculated. The ability of a chemical to bioaccumulate may be measured or estimated, and that property is called the bioaccumulation factor. For certain kinds of chemicals, fish consumption may deliver very high doses because of the high potential bioaccumulation of the chemicals in the fish. E-FAST uses the bioconcentration factor and estimates of the amount of fish eaten per person per day to predict the amount of chemical ingested by an individual on a daily basis.

Since an individual may ingest both drinking water and fish, there are multiple potential doses to evaluate. Assessments of chronic effects, such as cancer, require that long-term average concentrations be used. For SIC code assessments, E-FAST uses two stream flows from the distribution of stream flows for facilities in a given SIC code as the basis for calculations: mid-sized stream (50th percentile harmonic mean flow), and a small stream (10th percentile harmonic mean flow).

2.1.2.1 *Estimation of Drinking Water Exposures*

To estimate how much of a given chemical a person will ingest through drinking water obtained from rivers and streams, E-FAST uses Equations 2-6 through 2-8. E-FAST does not calculate potential drinking water exposures resulting from releases to estuaries and bays because these are not potable waters. Potential drinking water exposures are also not calculated for releases to lakes because of high uncertainty about appropriate dilution factors.

$$ADR_{POT} = \frac{SWC * (1 - DWT/100) * DWI * ED * CF1}{BW * AT} \qquad \text{(Eqn. 2-6)}$$

$$ADD_{POT} \text{ and } LADD_{POT} = \frac{SWC * (1 - DWT/100) * DWI * ED * Reldays * CF1}{BW * AT * (365 \text{ days/yr})} \qquad \text{(Eqn. 2-7)}$$

$$ADC \text{ and } LADC = \frac{SWC * (1 - DWT/100) * ED * Reldays * CF1}{AT * (365 \text{ days/yr})} \qquad \text{(Eqn. 2-8)}$$

where:

ADR_{POT}	=	Potential Acute Dose Rate (mg/kg/day);
ADD_{POT}	=	Potential Average Daily Dose (mg/kg/day);
$LADD_{POT}$	=	Potential Lifetime Average Daily Dose (mg/kg/day);
ADC	=	Average Daily Concentration in drinking water (mg/L);
LADC	=	Lifetime Average Daily Concentration in drinking water (mg/L);
SWC	=	Surface water concentration (ppb or μg/L);
DWT	=	Removal during drinking water treatment (%);
DWT/100	=	Converts drinking water treatment efficiency from a percentage to a fraction;
DWI	=	Drinking water intake rate (L/day);
Reldays	=	Days of chemical release per year;
BW	=	Body weight (kg);
ED	=	Exposure duration (30 years for ADC, LADC, ADD_{POT}, and $LADD_{POT}$; one day for ADR_{POT});
AT	=	Averaging time (30 years for ADD_{POT} and ADC; 75 years for $LADD_{POT}$ and LADC; one day for ADR_{POT}); and
CF1	=	Conversion factor of 0.001 mg/μg.

Stream flows used:

The **harmonic mean** stream flow is used to calculate the ADD_{POT}, $LADD_{POT}$, ADC, and LADC. The **30Q5** stream flow is used to calculate the ADR_{POT}. This is consistent with EPA Office of Water guidance (U.S. EPA, 1991).

What these equations do: Equations 2-6 and 2-7 convert an estimated surface water concentration to a drinking water exposure estimate. The surface water concentration (in µg/liter) is adjusted to account for any removal of the chemical during treatment of the drinking water and is then multiplied by the estimated drinking water ingestion rate in liters/day. The number of days of exposure over the time period of interest is calculated by multiplying the exposure duration by the number of release days per year. The factor of 0.001 converts from μg/ to mg. The product of these two calculations is then divided by body weight (in kg) and averaging time to yield mg/kg/day. The averaging times allow the calculation of average concentrations and average exposures over periods of time that include both days of release (and, consequently, exposure) and days without release. Average long-term drinking water ingestion rates are used to calculate chronic exposures. Ingestion rates for active individuals or high-end long-term average ingestion rates are used to calculate acute exposures.

2.1.2.2 *Estimating Exposures via Fish Ingestion*

To estimate how much of a given chemical a person will ingest through eating fish, E-FAST uses the following formulas:

$$ADR_{POT} = \frac{SWC * BCF * ED * FI\ Intake * CF1 * CF2}{BW * AT} \qquad \text{(Eqn. 2-9)}$$

$$ADD_{POT} \text{ and } LADD_{POT} = \frac{SWC * BCF * FI\ Intake * ED * Reldays * CF1 * CF2}{BW * AT * (365\ days/yr)} \qquad \text{(Eqn. 2-10)}$$

$$ADC \text{ and } LADC = \frac{SWC * BCF * ED * Reldays * CF1 * CF2}{AT * (365\ days/yr)} \qquad \text{(Eqn. 2-11)}$$

where:

ADD_{POT}	=	Potential Average Daily Dose (mg/kg/day);
ADR_{POT}	=	Potential Acute Dose Rate (mg/kg/day);
$LADD_{POT}$	=	Potential Lifetime Average Daily Dose (mg/kg/day);
ADC	=	Average Daily Concentration in fish tissue (mg/kg); and
LADC	=	Lifetime Average Daily Concentration in fish tissue (mg/kg).
SWC	=	Surface water concentration (ppb or µg/L);
BCF	=	Estimate of chemical's bioconcentration potential (L/kg);
FI intake	=	Fish Ingestion Rate (g/day);
Reldays	=	Days of chemical release per year;
BW	=	Body weight (kg);
ED	=	Exposure duration (30 years for ADC, LADC, ADD_{POT}, and $LADD_{POT}$; one day for ADR_{POT});
AT	=	Averaging time (30 years for ADC and ADD_{POT}; 75 years for LADC and $LADD_{POT}$; one day for ADR_{POT});
CF1	=	Conversion factor of 0.001 mg/μg; and

CF2 = Conversion factor of 0.001 kg/g.

What these equations do: Equations 2-9 and 2-10 convert an estimated surface water concentration to a fish ingestion exposure estimate. The harmonic mean stream flow is used to calculate all fish ingestion values. The distinction between acute and chronic fish ingestion is made on the basis of daily ingestion rate. Average long-term fish ingestion rates are used to calculate chronic exposures and average 1-day intakes are used to calculate acute fish ingestion exposures. This is in contrast to drinking water, where the distinction between acute and chronic values is made on the basis of both stream flows and ingestion values. The reason for this difference is that it takes time for chemical concentration to build up in fish; therefore, it is not appropriate to use a very low stream flow value, which occurs rarely, as the basis for calculating a chemical residue in fish.

2.2 Releases to Land

The term "releases to land" refers, in the context of E-FAST, to the direct disposal of the substance or manufacturing/processing wastes containing the substance to landfills or soil, or the indirect release to landfills or soil through the disposal of contaminated sludge created during the treatment of wastewater containing the substance. Chemicals are routinely sent to publicly owned treatment works (POTWs) for treatment. For those chemicals for which the extent of sorption to sludge is expected to be significant, it is possible that significant amounts of the substance could be released to land when the POTW sludge is disposed.

These releases are assessed because of the potential for migration of the substance through the soil column and into ground water. Once in the ground water, the substance may be drawn up through public and private wells for use as drinking water. Both of these types of releases can be assessed using E-FAST.

2.2.1 Estimation of Ground Water Concentrations from Landfill Releases

E-FAST uses a simple conservative method for estimating ground water concentrations that may result from chemical releases to landfills. These releases may be in the form of manufacturing/processing/commercial waste products deposited in a landfill or landfilled wastewater treatment plant sludge that contains the chemical. Maximum 70-year average groundwater concentrations are predicted using a derived relationship between annual release quantity and maximum 70-year average concentrations predicted by OPPT through a set of modeling exercises related to organic carbon/water partition coefficient (K_{oc}).

$$GWC = \frac{(Q) * (\text{migration factor})}{N} \qquad \text{(Eqn. 2-12)}$$

where:

GWC = Predicted 70-year average concentration in ground water (mg/L);
Q = Total chemical release rate to landfill (kg/yr for all sites);
N = Number of sites; and

Migration Factor = 2E-6 (log $K_{oc} \geq 4.5$), 3E-5 (log $K_{oc} \geq 2.5$ and < 4.5), 6E-5 (log $K_{oc} \geq 1.5$ and < 2.5), and 8E-5 (log $K_{oc} < 1.5$) (units = (mg/L)/(kg)).

The migration factors used in Equation 2-12 were derived using the results of an effort to model the fate of hypothetical non-volatile compounds (i.e., Henry's Law Constant of 1E-05 atm-m^3/mole) of varying soil sorption characteristics (i.e., log K_{oc} values ranging from 0 to 4.5) in soil types with different organic carbon contents and ground water hydraulic characteristics (GSC, 1987). The transport of the chemicals through the soil and ground water was modeled using SESOIL and AT123D, respectively. The loading of chemicals in a 1-hectare landfill was assumed to be 1,000 kg/year for 10 years. The distance to ground water was assumed to be 8 meters and the depth of a drinking water well 200 meters from the edge of the landfill was set at 20 meters.

The groundwater migration factors are expressed in the E-FAST program as "negligible" with a migration factor (MF) of zero; "negligible to slow," MF=2E-6; "slow," MF=3E-5; "moderate," MF=6E-5; and "rapid," MF=8E-5. These migration factors are assigned based on the corresponding K_{oc} values of the chemical being assessed as shown above in the definition of units in Equation 2-12.

2.2.2 Estimation of Drinking Water Exposures

To estimate how much of a given chemical a person will ingest through drinking groundwater, E-FAST uses Equation 2-13. Please note that it is not appropriate to use the groundwater migration factors described above to estimate acute exposures because the migration factors described in Section 2.2.1 were based on estimated 70-year average concentrations in ground water.

$$ADD_{POT} / LADD_{POT} = \frac{GWC * (1 - DWT/100) * DWI * EF * ED}{BW * AT * (365 \text{ days/yr})} \quad \text{(Eqn. 2-13)}$$

$$ADC / LADC = \frac{GWC * (1 - DWT/100) * EF * ED}{AT * (365 \text{ days/yr})} \quad \text{(Eqn. 2-14)}$$

where:

ADD_{POT}	=	Potential Average Daily Dose (mg/kg/day);
$LADD_{POT}$	=	Potential Lifetime Average Daily Dose (mg/kg/day);
GWC	=	Ground water concentration (mg/L);
ADC	=	Average Daily Concentration in drinking water (mg/L);
LADC	=	Lifetime Average Daily Concentration in drinking water (mg/L);
DWT	=	Removal during drinking water treatment (%);
DWT/100	=	Converts drinking water treatment efficiency from a percentage to a fraction;
DWI	=	Drinking water intake rate (L/day) (U.S. EPA, 1997);
EF	=	Exposure frequency (assumes 365 days/yr for all calculations);
BW	=	Body weight (adult) (kg) (U.S. EPA, 1997);
ED	=	Exposure duration (30 years for ADD_{POT} and $LADD_{POT}$); and

AT = Averaging time (30 years for ADC and ADD_{POT}; 75 years for LADC and $LADD_{POT}$).

2.3 Releases to Air

2.3.1 Estimation of Air Concentrations from Stack Releases

E-FAST uses a simple, conservative method for estimating ambient air concentrations that may result from air emissions from sources with tall stacks such as boilers and incinerators. Maximum annual average ground level air concentrations are predicted using a derived relationship ("generic ISCLT model method") between release amount and maximum annual average concentration that was developed by OPPT using Industrial Source Complex - Long Term (ISCLT) modeling of emissions from a hypothetical facility. This hypothetical facility has a stack height of 30 meters, a stack diameter of 1.5 meters, an exit gas temperature of 400 degrees K, and an exit velocity of 5 m/sec. The hypothetical facility was modeled using actual meteorological data for a city expected to produce relatively high concentrations, mostly because of the persistent wind directions in the area. The human receptor is assumed to be located 1,000 meters downwind from the stack because the ISCLT modeling showed that maximum concentrations occurred at this distance and because 1,000 meters is a reasonable distance from a facility with a tall stack at which one might expect residences to be located. The empirical relationship yielded by this modeling exercise is presented in Equation 2-15.

$$C = (Q_{yr}) * (3 \text{ x } 10^{-9}) \qquad \text{(Eqn. 2-15)}$$

where:

C = Predicted maximum annual average concentration in air (mg/m^3); and
Q_{yr} = Chemical release rate (kg/site-yr).

2.3.2 Estimation of Air Concentrations from Fugitive/Vent Releases

E-FAST uses a simple, conservative method for estimating ambient air concentrations from near-ground release sources such as process vents and local exhaust. Maximum annual average ground level air concentrations are predicted using the sector averaging form of the Gaussian algorithm presented in Turner (1970) (see Equation 2-16). Concentrations are predicted at the facility fenceline (assumed to be 100 meters downwind). Neutral atmospheric stability, an average wind speed of 5.5 m/sec, and wind direction toward the receptor 25 percent of the year are assumed. All emissions are assessed as coming from a single representative stack assumed to be 3 meters in height.

$$C = F * \left[\frac{(2.03 * (Q)}{(x) * (\sigma_z) * (\mu)}\right] * e^{[(-0.5) * (H/\sigma_2)^2]} \qquad \text{(Eqn. 2-16)}$$

where:

C	=	Predicted maximum annual average chemical concentration in air (mg/m^3);
F	=	Frequency wind blows toward receptor (conservatively assumed to be 25 percent);
Q	=	Chemical release rate (mg/sec);
X	=	Downwind distance of receptor (assumed to be 100 meters);
σ_z	=	Vertical dispersion coefficient (m). For 100 m downwind distance and neutral atmospheric stability, this value is 5 m (Turner, 1970). Neutral atmospheric stability occurs with the greatest frequency and is generally used to represent average long-term conditions;
μ	=	Mean wind speed (assumed to be 5.5 m/sec); and
H	=	Release height (assumed to be 3 m).

Using the default parameter values listed above for F, X, σ_z, μ, and H in Equation 2-16, causes Equation 2-16 to be reduced to Equation 2-17.

$$C = (Q) * (1.54 \times 10^{-4}) \qquad \text{(Eqn. 2-17)}$$

Equations 2-16 and 2-17 use units of mg/sec for Q. However, releases are generally provided in units of kg/yr. Assuming a continuous release (i.e., 24 hrs/day for 365 days/yr), kg/yr can be converted to mg/sec by the conversion factor 0.0317 (mg/sec)/(kg/yr). Thus, the revised Equation 2-17 is presented below as Equation 2-18.

$$C = (Q_{yr}) * (5 \times 10^{-6}) \qquad \text{(Eqn. 2-18)}$$

where:

C	=	Predicted maximum annual average concentration (mg/m^3); and
Q_{yr}	=	Chemical release rate (kg/site yr).

2.3.3 Estimation of Inhalation Exposures to Stack and Fugitive/Vent Releases

E-FAST uses the following equations to calculate exposures associated with stack releases. Please note that it is not appropriate to estimate acute exposures using this procedure because the factor described in Section 2.3.1 was based on estimated maximum annual average concentrations.

$$LADD_{POT} \text{ and } ADD_{POT} = \frac{(Q_{yr}) * (F) * (Factor) * (IR) * (ED)}{(BW) * (AT) * (365 \text{ days/yr})} \qquad \text{(Eqn. 2-19)}$$

$$\text{LADC and ADC} = \frac{(Q_{yr}) * (\text{Factor}) * (\text{ED})}{(\text{AT})} \quad \text{(Eqn. 2-20)}$$

where:

Q_{yr}	=	Chemical release rate (kg/site-yr);
F	=	Number of release days per year (days/yr) (assumed to be 365 days/yr);
Factor	=	3E-09 (mg-yr)/(m^3-kg) (derivation of the factor is explained in Section 2.3.1);
IR	=	Inhalation rate (m^3/day);
ED	=	Exposure duration (30 years for ADC, LADC, ADD_{pot} and $LADD_{pot}$);
BW	=	Body weight (kg); and
AT	=	Averaging time (30 years for ADD_{pot} and ADC; 75 years for $LADD_{pot}$ and LADC).

E-FAST uses the following equations to calculate exposures associated with fugitive/vent releases.

$$LADD_{pot} \text{ and } ADD_{pot} = \frac{(Q_{yr}) * (F) * (\text{Factor}) * (\text{IR}) * (\text{ED}) * (\text{CF1})}{(\text{BW}) * (\text{AT}) * (365 \text{ days/yr})} \quad \text{(Eqn. 2-21)}$$

$$\text{LADC and ADC} = \frac{(Q_{yr}) * (\text{Factor}) * (\text{ED})}{(\text{AT})} \quad \text{(Eqn. 2-22)}$$

where:

Q_{yr}	=	Chemical release rate (kg/site-yr);
F	=	Number of release days per year (days/yr);
Factor	=	5E-06 (mg-yr)/(m^3-kg) (derivation of this factor is explained in Section 2.3.2);
IR	=	Inhalation rate (m^3/day);
ED	=	Exposure duration (30 years for ADD_{pot}, ADC, $LADD_{pot}$, and LADC);
BW	=	Body weight (kg);
AT	=	Averaging time (30 years for ADD_{pot} and ADC; 75 years for $LADD_{pot}$ and LADC); and
CF1	=	Conversion factor of 1 day/24 hrs.

3. DOWN THE DRAIN

OPPT has developed a method for estimating concentrations of chemicals in surface waters that may result from the disposal of consumer products into household wastewater. The method assumes that household wastewater undergoes treatment at a local wastewater treatment facility and that treated effluent is subsequently discharged into surface waters. This estimation method also provides estimates of aquatic exposure and human exposure from ingestion of drinking water and fish that may become contaminated by these household wastewater releases. The method involves use of the Probabilistic Dilution Model (PDM), which allows an assessor to estimate the number of days per year that the concentration of chemical in surface water exceeds the level of concern for aquatic life.

Chemical constituents of some household products (e.g., detergents) are expected to end up in household wastewater. Chemical constituents of other household products are not likely to enter wastewater (e.g., fragrance in an air freshener). Prior to proceeding with the method(s) presented below, the physical-chemical properties and the functional role of the chemical in a product should be evaluated, since these properties could preclude the presence of the chemical in household wastewater.

The theoretical basis for estimating environmental releases of chemicals in household products is presented in this section. Included is the equation for estimating daily per capita wastewater releases and the consumer product-related input parameters required for this equation (Section 3.1); a discussion of the methods, inputs, and assumptions for estimating surface water concentrations (Section 3.2); potential dose rates from ingestion of drinking water and fish (Section 3.3); and a discussion of the assumptions and methods used to estimate probabilities of exceedence of concentrations of concern (Section 3.4).

3.1 Estimating Household Wastewater Releases

The equation for estimating the total daily per capita release of a chemical in household wastewater is as follows:

$$H_R = \frac{\text{ProdVol}}{\text{Pop}} * \frac{1000 \text{ grams}}{1 \text{ kg}} * \frac{1 \text{ year}}{365 \text{ days}} \qquad \text{(Eqn. 3-1)}$$

where:

H_R	=	Daily per capita release of the chemical to a wastewater treatment facility (grams/person/day);
ProdVol	=	Production volume (kg/year);
Pop	=	U.S. population (persons); and

The parameters required as input to Equation 3-1 are as follows:

(1) **U.S. Population**. The U.S. Census Bureau (U.S. Bureau of the Census, 1999) estimates the total U.S. population to be 2.727 x 10^8 persons. This value cannot be changed by the assessor.

(2) **Annual Production Volume**. This value is the mass of chemical produced annually or an estimate of the mass that is discharged annually to wastewater by consumers. This value is input by the assessor.

3.2 Method for Estimating Surface Water Concentrations

A screening-level estimate of the time-averaged surface water concentration of a chemical substance that may result from its release by a wastewater treatment facility receiving household wastewater can be calculated using the following equations:

$$C_{SM} = \frac{H_R * \frac{1}{Q_H} * (1 - WWT) * CF1}{SDF_M} \qquad \text{(Eqn. 3-2)}$$

$$C_{SH} = \frac{H_R * \frac{1}{Q_H} * (1 - WWT) * CF1}{SDF_L} \qquad \text{(Eqn. 3-3)}$$

where:

C_{SM} = Median time-averaged surface water concentration (μg/liter);
C_{SH} = High-end time-averaged surface water concentration (μg/liter);
H_R = Daily per capita release of chemical (i.e., pre-treatment release) (grams/person/day);
Q_H = Daily per capita wastewater volume released (364 L/person/day) (U.S. EPA, 1990; Versar, 1992c);
WWT = Fraction of chemical removed during wastewater treatment;
SDF_M = 50th percentile stream dilution factor for streams to which wastewater treatment facilities discharge (980.69) (Versar, 1992c);
SDF_L = 10th percentile stream dilution factor for streams to which wastewater treatment facilities discharge (75.44) (Versar, 1992c); and
CF1 = Conversion factor (1 x 10^6 μg/gram).

Each of the above factors and the assumptions on which they are based are discussed below. The underlying conservative assumption used in these equations is that all wastewater entering a wastewater treatment facility is from residential sources. With this assumption, the assessor can make use of readily available data to estimate concentrations of the chemical in ambient receiving waters.

(1) **<u>Daily household release of chemical (H_R)</u>**. This value, the pre-treatment release, is discussed in Section 3.1 and derived from Equation 3-1.

(2) **<u>Household wastewater volume released daily (Q_H)</u>**. The 1990 Needs data base was used to acquire statistics and distributions for per capita domestic flow (Versar, 1992c). These statistics are based on the subset of POTWs that have a domestic flow value and a resident-served population number. The subset is further restricted by deleting records that have domestic flow greater than total flows and records that are above the 95th percentile (assumed as erroneous outliers) of 885 liters per capita per day. The statistics are provided by total POTW flow categories and overall POTWs. Overall statistics and subset statistics (by flow category) are provided for all the records selected. The household wastewater flow of 364 liters/person/day was the 50th percentile value.

(3) **<u>Fraction of chemical removed during wastewater treatment (T)</u>**. Most chemicals in household wastewater can be expected to be removed to some extent during wastewater treatment. Chemical removal efficiency is dependent upon the physical--chemical properties of the chemical of concern and the extent of wastewater treatment (e.g., primary, secondary).

(4) **<u>Stream dilution factor (SDF_M, SDF_L)</u>**. The stream dilution factor (SDF_m, SDF_l) is equal to the volume of the receiving stream flow under mean flow conditions divided by the volume of the wastewater treatment facility effluent flow. Mean SDFs for wastewater treatment facilities based on 10th and 50th percentile values are presented in Table 6-1. These values were calculated for all active wastewater treatment facilities reported in the EPA STORET IFD file using the Stream Dilution Factor Program (Versar, 1992c). For the purpose of this effort, facilities with stream dilution factors of 1.0 or less were deleted; the SDFs presented in Table 3-1 are, therefore, the statistical distribution of SDFs based on those POTWs with SDFs greater than 1.0.

Table 3-1. Stream Dilution Factors for Publicly-Owned Treatment Works (POTWs)[a]

Percentile	Mean flow dilution factor
10th	75.44
50th	980.69

[a] The number of POTWs included in this analysis is 9,085; facilities with SDFs of 1.0 or less were deleted to generate this statistical distribution.

3.3 Method for Estimating Exposures from Ingestion of Drinking Water and Fish

This module generates estimates of potential acute and chronic exposures for the 50th and 10th percentile facility receiving streamflows. Potential lifetime average daily doses ($LADD_{POT}$) are calculated to represent chronic exposures to contaminated drinking water and fish over a lifetime. Acute potential dose rates (ADR_{POT}) are normalized to a shorter time period (i.e., one day). The EPA Guidelines for Exposure Assessment (U.S. EPA, 1992a) recommend that for estimating high-end exposures "not all factors should be set to values that maximize exposure or dose, since this will almost always lead to an estimate that is much too conservative." Consequently, potential dose rates are estimated by this module based on a combination of median and upper-end input values for the variables for which distribution data were available.

The variables used to calculate the $LADD_{POT}$ and ADR_{POT} include chemical concentration in surface water and intake rate. Median surface water concentrations are estimated in Equation 3-2 using the 50th percentile mean streamflow dilution factor. High-end surface water concentrations are estimated in Equation 3-3 using the 10th percentile mean streamflow dilution factor. Median and high-end intake rates for drinking water ingestion and fish ingestion are the same as those listed on Table 1-1 and used in the General Population Exposure from Industrial Releases module (see Section 2). Constant parameters include frequency of release from wastewater treatment facilities, averaging time, and body weight. User inputs include years of product usage and chemical-specific BCF.

Monte Carlo techniques were used to test the equations used for estimating central tendency and high-end, and bounding doses in this module. The analyses combined the data distributions for concentration and intake with other input parameters in the exposure algorithms used to calculate $LADDs_{POT}$ and $ADRs_{POT}$. Output distributions of $LADDs_{POT}$ and $ADRs_{POT}$ were developed based on 10,000 trials. The results of the Monte Carlo simulation indicated that point estimates based on all median inputs adequately represented central tendency outputs and point estimates based on all high-end inputs adequately represented bounding outputs. High-end dose estimates require that a combination of median and high-end inputs be used. The results of the Monte Carlo simulation indicated that for both drinking water exposure and fish ingestion exposure, combining high-end concentrations and median intake rates resulted in point estimates in the 90th percentile ranges of the Monte Carlo distributions. Thus, these input values were used in the high-end algorithms in the module. The equations used by the module for estimating ADR_{POT} and $LADD_{POT}$ from drinking water and fish ingestion exposure are presented in the sections below.

3.3.1 Drinking Water Exposure

A screening-level estimate of the drinking water potential dose rate to a chemical that may result from release of the substance by a wastewater treatment facility receiving household wastewater can be calculated using the following equations:

10th% surface water concentrations:

$$ADR_{POT} = \frac{C_{SH} * IR_{dm} * FQ * CF2}{(BW * AT)} \qquad \text{(Eqn. 3-5)}$$

$$ADD_{POT} \text{ and } LADD_{POT} = \frac{C_{SH} * IR_{dm} * FQ * CF2 * U}{(BW * AT * CF3)} \quad \text{(Eqn. 3-6)}$$

$$LADC \text{ and } ADC = \frac{C_{SH} * CF2 * U * FQ}{(AT * CF3)} \quad \text{(Eqn. 3-7)}$$

<u>50th% surface water concentrations</u>:

$$ADR_{POT} = \frac{C_{SM} * IR_{dm} * FQ * CF2}{(BW * AT)} \quad \text{(Eqn. 3-8)}$$

$$ADD_{POT} \text{ and } LADD_{POT} = \frac{C_{SM} * IR_{dm} * FQ * CF2 * U}{(BW * AT * CF3)} \quad \text{(Eqn. 3-9)}$$

$$LADC \text{ and } ADC = \frac{C_{SM} * CF2 * U * FQ}{(AT * CF3)} \quad \text{(Eqn. 3-10)}$$

where:

ADR_{POT}	=	Acute Potential Dose Rate from drinking water intake (mg/kg/day);
$LADD_{POT}$	=	Potential Lifetime Average Daily Dose from drinking water intake (mg/kg/day);
ADD_{POT}	=	Potential Average Daily Dose from drinking water intake (mg/kg/day);
ADC	=	Average Daily Concentration in drinking water (mg/L);
LADC	=	Lifetime Average Daily Concentration in drinking water (mg/L);
C_{SM}	=	50th% time-averaged surface water concentration (μg/liter);
C_{SH}	=	10th% time-averaged surface water concentration (μg/liter);
Ir_{dm}	=	Median volume of water consumed daily per person (liters/day);
FQ	=	Frequency of release from wastewater treatment facility (i.e., frequency of drinking contaminated water) (1 day for ADRs; 365 days/year for LADCs, ADCs, ADDs, and LADDs);
U	=	Years of product usage (i.e., years of potential exposure; conservative default assumption is 30 years);
BW	=	Body weight (adult), 71.8 kg;

AT	=	Averaging time (1 day for ADR_{POT}; 30 years for ADD_{POT} and ADC; and 75 years for $LADD_{POT}$ and LADC);
CF2	=	Conversion factor (1 x 10^{-3} mg/μg); and
CF3	=	Conversion factor (365 days/year).

The equation parameters that are not addressed in Table 1-1 are briefly discussed below.

(1) **Time-averaged surface water concentration (C_{SM}, C_{SH})**. The drinking water concentration of the chemical is assumed to be the same as the time-averaged surface water concentration under mean stream flow conditions as calculated using Equations 3-2 and 3-3 in Section 3.2. This conservative assumption implies that water is either ingested as raw stream water or, if treated before ingestion, that drinking water treatment removes none of the chemical.

(2) **Frequency of release from a wastewater treatment facility (FQ)**. This value reflects the frequency of consuming contaminated water and is a constant. It is set at 1 day for acute scenarios and 365 days per year for chronic scenarios.

(3) **Years of product usage (U)**. This value reflects the projected lifetime of a particular chemical product; a default value of 30 years is assumed.

3.3.2 Fish Ingestion Exposure

A screening-level estimate of the potential dose rate from ingestion of fish that may become contaminated with a chemical discharged by a wastewater treatment facility that receives household wastewater can be calculated using the following equations:

10th% surface water concentrations:

$$ADR_{POT} = \frac{C_{SH} * IR_{fm} * FQ * BCF * CF2 * CF4}{(BW * AT)} \qquad \text{(Eqn. 3-11)}$$

$$ADD_{POT} \text{ and } LADD_{POT} = \frac{C_{SH} * IR_{fm} * BCF * FQ * U * CF2 * CF4}{(BW * AT * CF3)} \qquad \text{(Eqn. 3-12)}$$

50th% surface water concentrations:

$$ADC \text{ and } LADC = \frac{C_{SH} * FQ * U * BCF * CF2}{(AT * CF3)} \qquad \text{(Eqn. 3-13)}$$

$$ADR_{POT} = \frac{C_{SM} * IR_{fm} * FQ * BCF * CF2 * CF4}{(BW * AT)} \qquad \text{(Eqn. 3-14)}$$

$$ADD_{POT} \text{ and } LADD_{POT} = \frac{C_{SM} * IR_{fm} * BCF * FQ * U * CF2 * CF4}{(BW * AT * CF3)} \qquad \text{(Eqn. 3-15)}$$

$$ADC \text{ and } LADC = \frac{C_{SM} * FQ * U * BCF * CF2}{(AT * CF3)} \qquad \text{(Eqn. 3-16)}$$

where:

ADR_{POT}	=	Acute Potential Dose Rate from fish ingestion (mg/kg/day);
$LADD_{POT}$	=	Potential Lifetime Average Daily Dose from fish ingestion (mg/kg/day);
ADD_{POT}	=	Potential Average Daily Dose from fish ingestion (mg/kg/day);
ADC	=	Average Daily Concentration in fish (mg/kg);
LADC	=	Lifetime Average Daily Concentration in fish (mg/kg);
C_{SM}	=	50th% time-averaged surface water concentration (μg/liter);
C_{SH}	=	10th% time-averaged surface water concentration (μg/liter);
Ir_{fm}	=	Median fish ingestion rate (grams/day);
BCF	=	Bioconcentration factor [mass of chemical/mass of fish per mass of chemical in water/liter of water (liters/kilogram)];
FQ	=	Frequency of release from a wastewater treatment facility (one day for ADRs, 365 days/year for ADC, LADC, ADD, and LADDs);
U	=	Years of product usage (i.e., years of potential exposure);
BW	=	Body weight of individual (kg);
AT	=	Averaging time (one day for ADRs, 30 years for ADCs and ADDs, 75 years for LADCs and LADDs);
CF2	=	Conversion factor (1 x 10^{-3} mg/μg);
CF3	=	Conversion factor (365 days/year); and
CF4	=	Conversion factor (1 x 10^{-3} kg/g).

With the exception of the Bioconcentration Factor (BCF), which is chemical-specific and must be provided by the user, all other equation parameters are discussed either in Section 3.3.1 or in Table 1-1.

3.4 Estimating Probability of Exceeding Concentrations of Concern

This module incorporates a modified version of PDM to calculate the number of days of exceedance of a surface water concentration of concern. This version:

(1) Only addresses publicly-owned treatment works (POTWs);

(2) Uses data from the 1990 Needs survey of POTWs;

(3) Uses a typical per capita loading (instead of discharge loading) to generate probabilities; and

(4) Accounts for POTW loadings and releases by using estimates of population served and estimates of per capita household releases.

The original PDM model uses facility effluent flow data from the EPA STORET Industrial Facilities Discharge (IFD) file and estimated W. E. Gates (WEG) stream flows from the GAGE file. The input dataset for this E-FAST module was produced in a different manner, as outlined below, to provide more complete and current POTW discharge and receiving stream flow data.

First, the reach numbers, POTW flows, and populations served were retrieved from the 1990 Needs survey for 15,349 POTWs having effluent flow data. The Needs survey data are updated biennially and represent a very comprehensive data base of POTW information (U.S. EPA, 1990).

Second, this data base was merged with the GAGE file in a somewhat different manner than the PDM files. To obtain the most realistic low flow value, both actual U.S. Geological Survey (USGS) and estimated WEG flows reported in GAGE were considered in the merge. For reaches with multiple reported stream flow values, the records were sorted in descending order of low stream flow, and the first observation was merged with the Needs reach. This method was used to eliminate potentially erroneously estimated flows (e.g., estimated low flows of zero).

Third, after extensive analysis and review of these data, it was decided to further eliminate records that had low stream flows that were less than the reported effluent flow values to that reach. Many of these records had reported low stream flow estimates of zero.

Finally, available population data (i.e., number of persons serviced by a POTW) were incorporated into the modified PDM model. POTW records that lacked population data were eliminated. The resulting dataset of 8,873 POTWs is used as the input dataset for PDM runs.

4. CONSUMER EXPOSURE

The Consumer Exposure Module (CEM) is an interactive model within E-FAST which calculates conservative estimates of potential inhalation exposure and potential and absorbed dermal exposure to chemicals in certain types of consumer products. CEM allows for screening-level estimates of acute potential dose rates, and average and lifetime average daily dose rates. Because the model incorporates either a combination of upper percentile and mean input values or all upper percentile input values for various exposure factors in the calculation of potential exposures/doses, the exposure/dose estimates are considered "high end" to "bounding" estimates.

Consumer inhalation exposures modeled in CEM use the same approach and calculations as the Multi-Chamber Concentration and Exposure Model (MCCEM) (Versar, 1997b), as well as scenarios depicted in the Screening -Level Consumer Inhalation Exposure Software (SCIES) (Versar, 1994). Dermal exposures are modeled using the same approach and equations as the DERMAL Exposure Model (Versar, 1995).

4.1 General Considerations for Estimation of Dermal Exposure

The dermal portion of CEM uses a film-thickness approach which assumes that exposure occurs from a thin layer of the consumer product on a defined skin surface area to determine potential exposure. Few data exist on the actual thickness of films of various products on human skin. Therefore, due to the uncertainty associated with the amount of product forming a film on the skin the dermal exposure estimates are considered less certain than those calculated in the inhalation portion of CEM. Absorbed dermal dose rates can be calculated using a permeability coefficient or a log octanol water coefficient, but these values and their use in calculating exposure also involves uncertainty. Absorbed exposure can only be calculated for the User-Defined Scenario in CEM.

CEM uses the "Surface Area to Body Weight Ratio (SA/BW)" rather than a dermally exposed surface area and body weight because there is a direct relationship between the surface area of an individual and their body weight. Combining surface area distributions with unrelated body weight data may lead to biases in estimating exposures (Phillips et. al., 1993). For example, combining an upper-percentile surface area value with a median or lower-percentile body weight could result in an unrealistic body type (i.e., an unrealistically tall individual).

4.2 Scenario Descriptions

General Purpose Cleaner (dermal and inhalation)- Exposure occurs from cleaning the outside of appliances and counter tops. The number of events per lifetime and the years per use were derived from the upper end values of cleaning events from the Household Cleaning Products Survey (Westat, 1987a). Professional judgement was then used in extrapolating this figure to a lifetime value. Six uses per week were assumed to occur for 50 weeks per year (one two-week vacation per year is also assumed to occur) for 57 years (between the ages of 18 and 75). The duration of use and the mass of the product used were derived from the Source Ranking Database (Versar, 1997a).

Interior Latex Paint (dermal and inhalation) - Exposure occurs from painting the rooms of a house. The value of 4 events per year was taken from the Household Solvent Products Survey

(Westat, 1987b). Professional judgement was used in assuming that these painting events would occur one year out of every five, producing a Years of Use value of 11 years over the course of 57 years (between the ages of 18 and 75). Default values for mass of product used and duration of use are also derived from the Household Solvent Products Survey (Westat, 1987b).

Fabric Protector (inhalation) - Exposure occurs from using a fabric protector on clothes and furniture in a house. The default values were derived from the Household Solvent Products Survey (Westat, 1987b).

Aerosol Paint (inhalation) - Exposure occurs from use of aerosol paint indoors for small paint jobs. The value of 6 events per year was taken from the Household Solvent Products Survey (Westat, 1987b). Professional judgement was used in assuming that these painting events would occur one year out of every five, producing a Years of Use value of 11 years over the course of 57 years (between the ages of 18 and 75). Default values for mass of product used and duration of use are also derived from the Household Solvent Products Survey (Westat, 1987b).

Liquid Laundry Detergent (**inhalation):** Exposure occurs from doing machine wash laundry at home. The number of events per lifetime and the years of use were derived from the Cleaning Products Survey (Westat, 1987a). The duration of use and the mass of the product used were derived from the Source Ranking Database (Versar, 1997a).

Liquid Laundry Detergent (dermal): Exposure occurs from hand washing delicate clothing. The frequency of use is once per week for 57 years (between the ages of 18 and 75) and is derived from the Household Cleaning Products Survey (Westat, 1987a). The SA/BW is derived from both hands being exposed. The film thickness was derived from the initial film thickness of water on the hands after initial immersion (Versar, 1992b). The dilution fraction was estimated from the dilution of ½ cup of detergent per use in a medium load.

Solid Air Freshener (inhalation) - Exposure occurs from using a solid air freshener in the home. The number of events per year is derived from replacing an air freshener every 60 days during the course of a year for 57 years (between the ages of 18 and 75). The individual is then passively exposed to the air freshener for the remaining days. The mass of product used was derived from the Source Ranking Database (Versar, 1997a). The duration of use values were derived by assuming a person is exposed to a solid air freshener for a minimum of 24 hours a day for 30 days and a maximum of 24 hours a day for 90 days before replacing the air freshener.

Bar Soap (dermal) - Exposure occurs from washing the whole body and hands during showering/ bathing and from washing the hands. The number of events is derived from five showers/baths per week between the ages of 1 and 16 and 65 and 75 (6,500 times/lifetime), one shower per day between the ages of 16 and 65 (17,836 times/lifetime), and two hand washes per day between the ages of 1 and 75 (54,020 times/lifetime). These usage rates produce a frequency of use for the body of 329 events per year and a frequency of use for the hands of 730 events per year for 74 years. The SA/BW was derived from the body and the hands being exposed. The film thickness was derived from the initial film thickness of bath oil/water mixture on the hands (Versar, 1992b). The dilution fraction was estimated from the monthly consumption of soap and the amount of water used to form lather (internal OPPT memorandum).

Used Motor Oil (dermal) - Exposure occurs from changing the oil in a car. The number of events is derived from the recommended length of time between oil changes (3 months), or 4 times a year for 57 years (between the ages of 18 and 75). The SA/BW is derived from the palms of both hands being exposed. The film thickness was derived from the uptake of mineral oil on the hands after immersion (Versar, 1992b). The dilution fraction is assumed to be full strength.

User Defined - Dermal and inhalation exposure occur from a user defined scenario. The user is responsible for providing all inputs. A secondary pop-up screen (see below) will query the user for the general product type (e.g., product applied to surface) being considered. The user may also select to calculate exposure using the film thickness approach to calculate potential dermal dose rates or the permeability coefficient method to calculate absorbed dermal dose rates.

If the user elects to calculate absorbed dermal dose rates, the user will have to input a permeability coefficient (Kp). The user has the option of selecting a permeability coefficient from a list of chemicals, entering the value directly, or calculating the value from a known octanol/water partition coefficient (Kow). Units for the permeability coefficient are cm/hr. More information on the permeability coefficient's relationship to Kow can be found in the Calculations section of Help.

4.3 Estimation of Indoor Air Concentrations

Indoor-air concentrations are predicted in the CEM model by implementing a deterministic, mass-balance calculation. A two-zone representation of a house is used, whereby the consumer product is assumed to be used in zone 1 (e.g., a kitchen) and zone 2 represents the remainder of the house. The modeled concentrations in the two zones are a function of the time-varying emission rate in zone 1, the volumes of zones 1 and 2, the air flows between each zone and outdoors, and the air flows between the two zones. For a conservative estimate of exposure, indoor sinks are assumed not to exist.

The model requires the conservation of pollutant mass as well as the conservation of air mass. The CEM model uses a set of differential equations whereby the time-varying concentration of the chemical in each zone is a function of the rate of pollutant loss and gain for that zone. These relationships can be expressed as follows (Sandberg, 1984):

A. Pollutant Mass Balance

$$\frac{\text{Change in Pollutant Mass}}{\text{Change in Time}} = \text{Production} \pm \text{Transport} - \text{Removal} \pm \text{Reactions} \qquad \text{(Eqn. 4-1)}$$

Neglecting reactions:

$$\frac{d\,\text{Mass}}{dt} = \Sigma\ \text{Sources} + \Sigma\ \text{Mass in} - \Sigma\ \text{Mass out} - \Sigma\ \text{Sinks} \qquad \text{(Eqn. 4-2)}$$

Or:

$$V_i \frac{dC_i}{dt} = \Sigma \text{ Sources} + \Sigma C_i Q_{ji} - \Sigma C_i Q_{ij} - \Sigma \text{ Sinks} \qquad \text{(Eqn. 4-3)}$$

where C refers to an air concentration, Q refers to a flow rate, V refers to the volume of the zone, and i and j refer to zones (there are two indoor zones plus outdoors). As noted above, sinks are ignored in the CEM model, but are shown here for completeness (Sandberg, 1984).

B. Air Mass Balance

$$\Sigma \text{ Flows into a zone} = \Sigma \text{ Flows out of a zone} \qquad \text{(Eqn. 4-4)}$$

Or:

$$\Sigma Q_{ji} = \Sigma Q_{ij} \qquad \text{(Eqn. 4-5)}$$

where Q, i and j are defined as above.

The flow rates are input as constants. The pollutant mass balance (Equation 4-3 above) is used in conjunction with the flow rates to predict the time-varying pollutant concentrations in each of the two indoor zones.

The differential equations can be solved by a variety of numerical solution techniques. The fourth-order Runge-Kutta method (also referred to as the Kutta-Simpson formula) is used for temporal integration (Mathews, 1992)). Although this method is not as computationally efficient as some others, it is very stable, self-starting, and accurate. The formula takes the following form (Mathews, 1992):

$$C(t + \ t) = C(t) + 1/6\,[K1 + 2\,K2 + 2\,K3 + K4] \qquad \text{(Eqn. 4-6)}$$

where:

$$K1 = \frac{dC}{dt}(\ t), \text{ evaluated at time} = t,\ C = C(t)$$

$$K2 = \frac{dC}{dt}(\ t), \text{ evaluated at time} = t + (\ t)/2,\ C = C(t) + K1/2$$

$$K3 = \frac{dC}{dt}(\ t), \text{ evaluated at time} = t + (\ t)/2,\ C = C(t) + K2/2$$

$$K4 = \frac{dC}{dt}(\ t), \text{ evaluated at time} = t + (\ t),\ C = C(t) + K3.$$

The Runge-Kutta technique has been evaluated for stability over a wide range of values for time step, zone volumes, and flow rates.

The manner in which chemical emissions from a product are represented in the CEM model is dependent upon how the product is used and its chemical makeup. In general, the emissions are varied over time using a formula that accounts for the manner in which the product is used or applied, the total applied mass of the product, the weight fraction of the chemical in the product, and the molecular weight and vapor pressure of the chemical.

For a "Product Applied to Surface," such as a general purpose cleaner or a latex paint, an incremental source model is used. This model assumes a constant application rate over the user-specified duration of use; each instantaneously applied segment has an emission rate that declines exponentially over time, at a rate that depends on the chemical's molecular weight and vapor pressure.

In the case of a general purpose cleaner, the equation for exponentially declining emissions for each instantaneously applied segment is as follows:

$$E(t) = E(0) * \exp(-kt) \qquad \text{(Eqn. 4-7)}$$

where E (t) is the emission rate (mass/time) at time t (in hours), E (0) is the initial emission rate at time 0, k is a first-order rate constant for the emissions decline (inverse hours), and t is elapsed time (hours). The value of k is determined from an empirical relationship, developed by Chinn (1981), between the time (in hours) required for 90 percent of a pure chemical film to evaporate (EvapTime) and the chemical's molecular weight (MW) and vapor pressure(VP):

$$\text{EvapTime} = 145 / (\text{MW} * \text{VP})0.9546 \qquad \text{(Eqn. 4-8)}$$

The value of k is determined from the 90-percent evaporation time as follows:

$$k = \ln(10) / \text{EvapTime} \qquad \text{(Eqn. 4-9)}$$

E (0) can be determined from the fact that the integral of Equation 4-7, which accounts for all chemical mass released, is equal to E (0) / k. However, the equation for the total emission profile resulting from the combination of constant application and exponentially declining emissions (see g) requires knowledge only of the total mass released and k.

Latex paint is handled much like a general purpose cleaner, with two exceptions: (1) a double exponential model is used to account for an initial "fast" release that is governed primarily by evaporation, followed by a "slow" release dominated by diffusion; and (2) only 25 percent of the applied mass is released, as a substantial fraction of the mass becomes "trapped" in the painted substrate when it dries. Empirical studies reported by Wilkes et al. (1996) support the assumption of 25 percent mass released and have estimated a relationship between the "fast" rate of decline (k1) and vapor pressure (VP), and between the "slow" rate of decline and molecular weight (MW):

$$k1 = 233.25 * VP \qquad \text{(Eqn. 4-10)}$$
$$k2 = 0.0000584 * MW$$

The equation for the resultant emission profile requires estimates of the total mass released, k1 and k2, and the fraction of released mass associated with the first exponential (Evans, 1994). Based on the empirical studies reported by Wilkes, et al. (1996), CEM associates 10 percent of the released mass with the first exponential.

For a "Product Sprayed on Surface," such as a fabric protector or an aerosol paint, a portion (default of 1%) is assumed to be aerosolized and is therefore immediately available for uptake by inhalation. The remainder is assumed to contact the target surface, and to subsequently volatilize at a rate that depends upon the chemical's molecular weight and vapor pressure.

The constant emission rate (ER, in mass/time) for the aerosolized potion is as follows:

$$ER = (\text{Applied Mass} * \text{Fraction Aerosolized}) / \text{Duration of Product Use} \qquad \text{(Eqn. 4-11)}$$

The remaining (non-aerosolized) mass is treated in the same manner as described above for a general purpose cleaner, combining a constant application rate with an exponentially declining rate for each instantaneously applied segment.

For a "Product Added to Water," such as a laundry detergent, the chemical is assumed to emit at a constant rate over a duration that depends on its molecular weight and vapor pressure. If this duration is longer than the user-specified duration of use, then the chemical emissions are truncated at the end of the product-use cycle (i.e., in the case of a washing machine, the remaining chemical mass is assumed to go "down the drain").

The potential duration of emissions in this case is determined from the chemical’s 90-percent evaporation time, determined as given above in Equation 4-8. The constant emission rate (ER) is

$$(ER) = \text{Mass} / \text{EvapTime} \qquad \text{(Eqn. 4-12)}$$

It is possible, however, for EvapTime to be longer than the duration of product use. In that case, the emission rate in Equation 4-12 is applied only through the end of the use cycle, resulting in loss of some mass “down the drain” before EvapTime is reached.

For a "Product Placed in Environment," such as a solid air freshener, the chemical is assumed to emit at a constant rate over a duration that depends on its molecular weight and vapor pressure. If this duration exceeds the user-specified duration of use, then the chemical emissions are truncated at the end of the product-use period, because the product is assumed to be removed from the house after the use period. Equation 4-12 applies equally here, with the loss of some mass when EvapTime is longer than the use cycle.

In certain cases the above source models could lead to predicted concentrations that exceed the chemical's saturation concentration in air. However, the model adjusts the time-varying emission rate so that the saturation concentration is never exceeded. In such cases, the chemical mass will be released at a slower rate than implied by the above source models, once the saturation concentration is reached. The same chemical mass ultimately will be released, except in cases where emissions are truncated at the end of the product-use period.

The following equation is used to estimate the value for the saturation concentration:

$$Csat = (VP/760 \text{ mm Hg/atm} * MW * 1000 \text{ mg/g} * 1000 \text{ L/m}^3) / (R * T) \qquad \text{(Eqn. 4-13)}$$

where:

Csat	=	saturation concentration (mg/m^3);
VP	=	vapor pressure (mm Hg);
MW	=	molecular weight (g/mole);
R	=	gas constant = 0.0821 liter atm/mole °K; and
T	=	temperature of the air (°K).

At each time step CEM checks whether the current value for the emission rate results in an indoor concentration that exceeds Csat. If so, then the emission rate is reduced to a value that results in the indoor concentration equaling Csat. In such a case, CEM keeps track of the cumulative mass that has been "subtracted" to meet the Csat constraint; release of this accumulated "excess" mass is initiated at a later point in time, when the modeled concentration otherwise would be below the Csat value. This procedure is continued until all excess mass has been released, unless the end of the time period for the model run is encountered first.

4.4 Estimation of Consumer Exposures

4.4.1 Estimation of Inhalation Exposures

Three different inhalation exposure calculations are performed in the CEM model: the Lifetime Average Daily Potential Dose ($LADD_{pot}$) calculation; the Average Daily Potential Dose (ADD_{pot}) calculation; and the Acute Potential Dose Rate (ADR_{pot}) calculation.

In general, each uses the following equation to calculate its result:

$$\text{Dose} = \frac{C * IR * FQ * D * Y * WF}{BW * AT * (365 \text{ days/yr})} \qquad \text{(Eqn. 4-14)}$$

where:

C	=	Exposure concentration (mg/m^3);
IR	=	Inhalation rate (m^3/hr);
FQ	=	Frequency (events/year);
D	=	Duration of an event (hours/event);
Y	=	Years of use (years);
WF	=	Weight fraction (unitless);
BW	=	Body weight (kilograms); and

AT	=	Averaging time (57 years for ADD_{pot}; 75 years for $LADD_{pot}$; one day for ADR_{pot}).

The exposure concentration for the inhalation model is calculated iteratively, taking into account the vapor pressure of the chemical, its mass, its weight fraction, the house and zone volumes, the air exchange rate, the inhalation rates during and after use, and the exposed individual's activity patterns during and after use.

The weight fraction term in the above calculations varies. For the $LADD_{pot}$ and the ADD_{pot} calculations, the median weight fraction, exposure duration, and mass of product used are used. In the ADR_{pot} calculation, the 90th percentile weight fraction, exposure duration, and mass of product used are used. Default values for the weight fractions come from the Source Ranking Database (Versar, 1997a).

Three different inhalation concentration calculations are performed in CEM: Lifetime Average Daily Concentration (LADC); Average Daily Concentration (ADC); and Peak Concentration (Cpeak). The LADC and ADC calculations use the following equation (which is part of Eqn. 5-14):

$$\text{Concentration} = \frac{TC * FQ * Y * WF}{AT * 365 \text{ days/yr}} \qquad \text{(Eqn. 4-15)}$$

where:

TC	=	Time-integrated air concentration per product-use event (mg/m^3-days/event);
FQ	=	Frequency (events/year);
Y	=	Years of use (years);
WF	=	Weight fraction (unitless); and
AT	=	Averaging time (57 years for ADD_{pot}; 75 years for $LADD_{pot}$; one day for ADR_{pot}).

The peak concentration is the highest instantaneous air concentration that is modeled during the exposure event.

4.4.2 Estimation of Dermal Exposures

Three different dermal exposure calculations are performed in the CEM model: the Lifetime Average Daily Potential Dose ($LADD_{pot}$) calculation; the Average Daily Potential Dose (ADD_{pot}) calculation; and the Acute Potential Dose Rate (ADR_{pot}) calculation.

In general, each uses the following equation to calculate its result:

$$\text{Dose} = \frac{Q * SA/BW * FQ * Y * WF * 1000 \text{ mg/g}}{AT * (365 \text{ days/yr})} \qquad \text{(Eqn. 4-16)}$$

where:

Q	=	Amount retained on the skin (grams/square centimeter-event);
SA/BW	=	Surface area to body weight ratio (square centimeter/kilogram);
FQ	=	Frequency of use (events/year);
Y	=	Years of use (years);
WF	=	Weight fraction of product (unitless); and
AT	=	Averaging time (57 years for ADD_{pot}; 75 years for $LADD_{pot}$; one day for ADR_{pot}).

In the dermal calculations for Bar Soap, the SA/BW term and the FQ term is split into two terms, a SA/BW and FQ for the body and a SA/BW and FQ for the hands. The dose for the body and hands is calculated and then summed to provide an overall dose for Bar Soap.

The weight fraction term in the above calculations varies. For the LADD and the ADD calculations, the median weight fraction is used. In the APDR calculation, the 90th percentile weight fraction is used. Default values for the weight fractions come from the Source Ranking Database (e).

The above calculations are performed for scenarios to calculate the **potential** dose. Potential dose is the amount a chemical contained in bulk material applied to the skin. In the User Defined Scenario the user may select to calculate **absorbed** dermal exposure using the permeability coefficient method. Absorbed dose is the amount of substance penetrating across the absorption barriers of an organism. The user has the option of choosing a permeability coefficient by one of three methods

- entering a permeability coefficient,
- selecting a permeability coefficient value from a list of common chemicals,
- entering a Kow value and having the model calculate the permeability coefficient using the following equation (U.S. EPA, 1992b):

$$\log (Kp) = -2.72 + 0.71 * \log (Kow) - 0.0061 * MW \qquad \text{(Eqn. 4-17)}$$

where:

Kp	=	Permeability coefficient (centimeter/hour);
Kow	=	Octanol/water partition coefficient (unitless); and
MW	=	Molecular weight (g/mole).

The permeability coefficient is then entered into the following equation to calculate dermal exposure

$$Dose = \frac{Kp * ED * Dil * Den * SA/BW * FQ * Y * WF * 1000\ mg/g}{AT * 365\ days/year} \qquad \text{(Eqn. 4-18)}$$

where:

Kp	=	Permeability coefficient (centimeter/hour);
ED	=	Exposure duration (hour/event);
Dil	=	Dilution (unitless);
Den	=	Density (gram/cubic centimeter);
SA/BW	=	Surface area to body weight ratio (square centimeter/kilogram);
FQ	=	Frequency of use (events/year);
Y	=	Years of use (years);
WF	=	Weight fraction of product (unitless); and
AT	=	Averaging time (57 years for ADD_{pot}; 75 years for $LADD_{pot}$; one day for ADR_{pot}).

5. AQUATIC ENVIRONMENT EXPOSURE/RISK

An important assessment issue for releases to surface water is the effect that a chemical may have on aquatic organisms, from algae to fish. If the food chain is impacted in a stream, the consequences can be deleterious to the health of the stream. A healthy stream with many organisms will have a better ability to handle chemical releases than one whose quality is already compromised. The organisms lower on the food chain, such as algae, tend to have shorter lives, making shorter exposure time periods more critical. Since in-stream concentrations will vary with the stream flow, there may be periods of lower flow conditions when the same amount released on a regular basis may cause problems. E-FAST relies on historical stream flow data to predict how often this will happen under "local" and "generic" exposure settings.

The Probabilistic Dilution Model (PDM) unlike simple dilution calculations, attempts to account for the natural variability of stream flows and effluent flows when comparing concentration values to concern levels. To account for the variability, a probability distribution of stream flows is incorporated into the simple dilution calculation. It is this difference that permits the assessor to estimate the days of exceedance of a concern concentration (i.e., for the protection of aquatic life) for a chemical.

Before the user can perform an analysis using PDM, he/she must have some knowledge of the following:

- The type of analysis the assessor desires - a site specific or generic Standard Industrial Classification (SIC) code category;
- The reach number (eleven digit number that identifies the stream segment) or SIC code category;
- The loading of the chemical (i.e., kilograms of chemical released to water per day of discharge);
- Number of release days per year of the chemical; and
- The concern concentration of the chemical.

The resulting output would then be:

- The percentage of days per year the concern concentration is exceeded (i.e., the number of days of exceedance divided by 365 days per year); and
- The number of days the concern concentration is exceeded per year.

General explanations of the options available in PDM are provided in the following four subsections. Section 5.5 describes situations for which PDM is not appropriate.

5.1 OPTION 1: Analysis of Reaches with USGS Gaging Stations

This option uses measured flow data from the USGS gaging station located on the reach. Only USGS gaging stations with at least 100 daily flow values for the period of record when PDM was developed in the late 1980s were included in PDM. This minimum number was required to create a percentile distribution for the reach of interest. The percentile flows are stored in a file for the reach, to be accessed when exceedances are to be estimated.

The output of PDM is calculated as follows for this option:

(1) Calculate the stream concentration for each percentile flow by dividing the loading by each individual flow value. This is simple dilution.

(2) Compare the concern concentration to the 100 calculated stream concentrations. Select the highest percentile flow that yields a concentration greater than the concern concentration.

(3) Calculate the percent of year exceeded and days per year exceeded.

5.2 OPTION 2: Analysis of Reaches without USGS Gaging Stations

For many reaches, fewer than 100 daily flows were available when PDM was developed in the late 1980s. This occurred because no USGS gaging station was located on the reach or the gaging station present had fewer than 100 daily flow values. For these reaches, PDM accesses and uses the mean and low (7Q10) flows estimated by EPA's Office of Water for the specified reach and a coefficient of variation of stream flow calculated by PDM for the specified reach. The coefficient of variation is calculated using a previously developed regression equation for the subbasin of interest and the 7Q10 to mean flow ratio for the specified reach.

From here, a series of probability calculations are performed to compute the probability that the downstream concentration will exceed a concern concentration. These calculations involve the mean and coefficient of variation for the stream flow as well as the effluent flow and effluent concentration.

5.3 OPTION 3: SIC Code Category, Reasonable Worst Case Analysis

For this type of analysis the probability of exceedance of a concern concentration is calculated in a similar manner as for Option 2, reaches without gaging stations. However, the run time for such calculations on numerous facilities and reaches within an SIC code grouping was much too long for use in a PC environment when PDM was developed in the late 1980s.

Instead, matrix files were created that contain the probabilities calculated on EPA's mainframe computer for predetermined values of concern concentration and amount of chemical released. The resulting matrix files were stored on the PC for use. For concern level/loading rate ratios that are not represented in the matrix, an interpolation program was added to estimate the probability using the ratio of the values entered by the user to a value in the matrix.

The matrix files contain the average of the sum of the highest 10th percentile probabilities for a particular concern concentration to loading ratio. That is, if there were 300 facilities in an SIC-code grouping, the probability of exceedance was generated for all 300 facilities but only the top 30 exceedance values were summed, averaged, and stored on the PC. This analysis is considered reasonable worst case because the highest probabilities of exceedance are used rather than all probabilities.

5.4 OPTION 4: SIC Code Category, Average Case Analysis

In this case, matrix files were created in the same manner as in option 3. After all of the probabilities were calculated, they all were summed, averaged, and stored. Therefore, the probabilities of exceedance for all facilities are used.

5.5 What PDM Does Not Cover

There are some release situations for which PDM is not appropriate. PDM does not generate exceedances for substances released to still waters such as bays and estuaries. In this case, a dilution factor approach is used. The amount of material discharged is divided by the plant flow to generate an effluent concentration. The effluent concentration is further diluted once it is discharged into the waterbody. This is accounted for via the use of acute and chronic dilution factors.

For example, if the effluent concentration is 20 ppb and the (unitless) acute and chronic dilution factors are 2 and 10, respectively, the estimated concentrations in surface water are 10 ppb (acute) and 2 ppb (chronic). The concentration of concern, which is a chronic value, is compared with the chronic stream concentration, in this case 2 ppb. This concentration is assumed to occur every day of release. Therefore, if the chronic stream concentration is 2 ppb, the release occurs for 50 days per year, and the concern concentration is 1 ppb, we would assume 50 days of exceedance of the concentration of concern.

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